Gromov-Hausdorff Approximation of Metric Spaces with Linear Structure

Frédéric Chazal, Jian Sun

Gromov-Hausdorff Approximation of Metric Spaces with Linear Structure

Frédéric Chazal [*], Jian Sun [†]

May 6, 2013

Abstract

In many real-world applications data come as discrete metric spaces sampled around 1-dimensional filamentary structures that can be seen as metric graphs. In this paper we address the metric reconstruction problem of such filamentary structures from data sampled around them. We prove that they can be approximated, with respect to the Gromov-Hausdorff distance by well-chosen Reeb graphs (and some of their variants) and we provide an efficient and easy to implement algorithm to compute such approximations in almost linear time. We illustrate the performances of our algorithm on a few synthetic and real data sets.

1 Introduction

Motivation. With the advance of sensor technology, computing power and Internet, massive amounts of geometric data are being generated and collected in various areas of science, engineering and business. As they are becoming widely available, there is a real need to analyze and visualize these large scale geometric data to extract useful information out of them. In many cases these data are not embedded in Euclidean spaces and come as (finite) sets of points with pairwise distances information, i.e. (discrete) metric spaces. A large amount of research has been done on dimensionality reduction, manifold learning and geometric inference for data embedded in, possibly high dimensional, Euclidean spaces and assumed to be concentrated around low dimensional manifolds [5, 29, 34]. However, the assumption of data lying on a manifold may fail in many applications. In addition, the strategy of representing data by points in Euclidean space may introduce large metric distortions as the data may lie in highly curved spaces, instead of in flat Euclidean space raising many difficulties in the analysis of metric data. In the past decade, with the development of topological methods in data analysis, new theories such as topological persistence (see, for example, [21, 36, 8, 10]) and new tools such as the Mapper algorithm [33] have given rise to new algorithms to extract and visualize geometric and topological information from metric data without the need of an embedding into an Euclidean space. In this paper we focus on a simple but important setting where the underlying geometric structure approximating the data can be seen as a branching filamentary structure i.e., more precisely, as a *metric graph* which is a topological graph endowed with a length assigned to each edge (see Section 2). Such structures appear naturally in various real-world data such as collections of GPS traces collected by vehicles on a road network, earthquakes distributions that concentrate around geological faults, distributions of galaxies in the universe, networks of blood vessels in anatomy or hydrographic networks in geography just to name a few of them. It is thus appealing to try to capture such filamentary structures and to approximate the data by metric graphs that will summarize the metric and allow convenient visualization.

[*] INRIA Saclay - France - frederic.chazal@inria.fr
[†] Tsinghua University - China

Contribution In this paper we address the metric reconstruction problem for filamentary structures. The input of our method and algorithm is a metric space (X, d_X) that is assumed to be close with respect to the so-called Gromov-Hausdorff distance d_{GH} to a much simpler, but unknown, metric graph $(G', d_{G'})$. Our algorithm outputs a metric graph (G, d_G) that is proven to be close to (X, d_X). Our approach relies on the notion of Reeb graph (and some variants of it introduced in Section 3.1) and one of our main theoretical result can be stated as follows.

Theorem 3.10. *Let (X, d_X) be a compact connected geodesic space, let $r \in X$ be a fixed base point such that the metric Reeb graph (G, d_G) of the function $d = d_X(r, .) : X \to \mathbb{R}$ is a finite graph. If for a given $\varepsilon > 0$ there exists a finite metric graph $(G', d_{G'})$ such that $d_{GH}(X, G') < \varepsilon$ then we have*

$$d_{GH}(X, G) < 2(\beta_1(G) + 1)(17 + 8N_{E,G'}(8\varepsilon))\varepsilon$$

where $N_{E,G'}(8\varepsilon)$ is the number of edges of G' of length at most 8ε and $\beta_1(G)$ is the first Betti number of G, i.e. the number of edges to remove from G to get a spanning tree. In particular if X is at distance less than ε from a metric graph with shortest edge larger than 8ε then $d_{GH}(X, G) < 34(\beta_1(G) + 1)\varepsilon$.

Turning this result into a practical algorithm requires to address two issues:

- First, raw data usually do not come as geodesic spaces. They are given as discrete sets of point (and thus not connected metric spaces) sampled from the underlying space (X, d_X). Moreover in many cases only distances between nearby points are known. A geodesic space (see Section 2 for a definition of geodesic space) can then be obtained from these raw data as a neighborhood graph where nearby points are connected by edges whose length is equal to their pairwise distance. The shortest path distance in this graph is then used as the metric. In our experiments we use this new metric as the input of our algorithm. The question of the approximation of the metric on X by the metric induced on the neighborhood graphs is out of the scope of this paper.

- Second, approximating the Reeb graph (G, d_G) from a neighborhood graph is usually not obvious. If we compute the Reeb graph of the distance function to a given point defined on the neighborhood graph we obtain the neighborhood graph itself and do not achieve our goal of representing the input data by a simple graph. It is then appealing to build a two dimensional complex having the neighborhood graph as 1-dimensional skeleton and use the algorithm of [27, 31] to compute the Reeb graph of the distance to the root point. Unfortunately adding triangles to the neighborhood graph may widely change the metric between the data points on the resulting complex and significantly increase the complexity of the algorithm. We overcome this issue by introducing a variant of the Reeb graph, the α-Reeb graph, inspired from [33] and related to the recently introduced notion of graph induced complex [14], that is easier to compute than the Reeb graph but also comes with approximation guarantees (see Theorem 3.11). As a consequence our algorithm relies on the Mapper algorithm of [33] and runs in almost linear time (see Section 4).

Related work. Approximation of data by 1-dimensional geometric structures has been considered by different communities. In statistics, several approaches have been proposed to address the problem of detection and extraction of filamentary structures in point cloud data. For example Arial-Castro et al [4] use multiscale anisotropic strips to detect linear structure while [24, 23] and more recently [25] base their approach upon density gradient descents or medial axis techniques. These methods apply to data corrupted by outliers embedded in Euclidean spaces and focus on the inference of individual filaments without focus on the global geometric structure of the filaments network.

In computational geometry, the curve reconstruction problem from points sampled on a curve in an euclidean space has been extensively studied and several efficient algorithms have been proposed [3, 16, 17]. Unfortunately, these methods restricts to the case of simple embedded curves (without singularities or self-intersections) and hardly extend to the case of topological graphs. In a more intrinsic setting where data come as finite abstract metric spaces, [1] propose an algorithm that outputs, under some specific sampling conditions, a topologically correct (up to a homeomorphism) reconstruction of

the approximated graph. However this algorithm requires some tedious parameters tuning and relies on quite restrictive sampling assumptions. When these conditions are not satisfied, the algorithm may fail and not even outputs a graph. Compared to the algorithm of [1], our algorithm not only comes with metric guarantees but also whatever the input data is, it always outputs a metric graph and does not require the user to choose any parameters. Our approach is also related to the so-called Mapper algorithm [33] that provides a way to visualize data sets endowed with a real valued function as a graph. Indeed the implementation of our algorithm relies on the Mapper algorithm where the considered function is the distance to the chosen root point. However, unlike the general mapper algorithm, our methods provides an upper bound on the Gromov-Hausdorff distance between the reconstructed graph and the underlying space from which the data points have been sampled.

In theoretical computer science, there is much of work on approximating metric spaces using trees [7, 2, 12] or distribution of trees [18, 22] where the trees are often constructed as spanning trees possibly with Steiner points. Our approach is different as our reconstructed graph or tree is a quotient space of the original metric space where the metric only gets contracted (see Lemma 3.6). Finally we remark that the recovery of filament structure is also studied in various applied settings, including road networks [11, 35], galaxies distributions [13].

The paper is organized as follows. The basic notions and definitions used throughout the paper are recalled in Section 2. The Reeb and α-Reeb graphs endowed with a natural metric are introduced in Section 3.1 and the approximation results are stated and proven in Sections 3.2 and 3.3. Our algorithm is described in Section 4 and experimental results are presented and discussed in Section 5.

2 Preliminaries: metric spaces, metric graphs and Gromov-Hausdorff distance

Recall that a metric space is a pair (X, d_X) where X is a set and $d_X : X \times X \to \mathbb{R}$ is a non negative map such that for any $x, y, z \in X$, $d_X(x, y) = 0$ if and only if $x = y$, $d_X(x, y) = d_X(y, x)$ and $d_X(x, z) \leqslant d_X(x, y) + d_X(y, z)$. Two compact spaces (X, d_X) and (Y, d_Y) are isometric if there exits a bijection $\varphi : X \to Y$ that preserves the distances, namely: for any $x, x' \in X, d_Y(\varphi(x), \varphi(x')) = d_X(x, x')$. The set of isometry classes of compact metric spaces can be endowed with a metric, the so-called Gromov-Hausdorff distance that can be defined using the following notion of correspondence ([6] Def. 7.3.17).

Definition 2.1. Let (X, d_X) and (Y, d_Y) be two compact metric spaces. Given $\varepsilon > 0$, an *ε-correspondence* between (X, d_X) and (Y, d_Y) is a subset $C \subset X \times Y$ such that:
i) for any $x \in X$ there exists $y \in Y$ such that $(x, y) \in C$;
ii) for any $y \in Y$ there exists $x \in X$ such that $(x, y) \in C$;
iii) for any $(x, y), (x', y') \in C$, $|d_X(x, x') - d_Y(y, y')| \leqslant \varepsilon$.

Definition 2.2. The *Gromov-Hausdorff distance* between two compact metric spaces (X, d_X) and (Y, d_Y) is defined by

$$d_{GH}(X, Y) = \frac{1}{2} \inf\{\varepsilon \geqslant 0 : \text{there exists an } \varepsilon\text{-correspondence between } X \text{ and } Y\}$$

A metric space (X, d_X) is a *path metric space* if the distance between any pair of points is equal to the infimum of the lengths of the continuous curves joining them [1]. Equivalently (X, d_X) is a path metric space if and only if for any $x, y \in X$ and any $\varepsilon > 0$ there exists $z \in X$ such that $\max(d_X(x, z), d_X(y, z)) \leqslant \frac{1}{2} d_X(x, y) + \varepsilon$ [26]. In the sequel of the paper we consider compact path metric spaces. It follows from the Hopf-Rinow theorem (see [26] p.9) that such spaces are *geodesic*, i.e.

[1] see [26] Chap.1 for the definition of the length of a continuous curve in a general metric space

for any pair of point $x, x' \in X$ there exists a minimizing geodesic joining them.[2] A continuous path $\delta : I \to X$ where I is a real interval or the unit circle is said to be *simple* if it is not self intersecting, i.e. if δ is an injective map.

Recall that a *(finite) topological graph* $G = (V, E)$ is the geometric realisation of a (finite) 1-dimensional simplicial complex with vertex set V and edge set E. If moreover each 1-simplex $e \in E$ is a metric edge, i.e. $e = [a, b] \subset \mathbb{R}$, then the graph G inherits from a metric d_G which is the unique one whose restriction to any $e = [a, b] \in E$ coincides with the standard metric on the real segment $[a, b]$. Then (G, d_G) is a *metric graph* (see [6], Section 3.2.2 for a more formal definition). Intuitively, a metric graph can be seen as a topological graph with a length assigned to each of its edges.

The *first Betti number* $\beta_1(G)$ of a finite topological graph G is the rank of the first homology group of G (with coefficient in a field, e.g. $\mathbb{Z}/2$), or equivalently, the number of edges to remove from G to get a spanning tree.

3 Approximation of path metric spaces with Reeb-like graphs

Let (X, d_X) be a compact geodesic space and let $r \in X$ be a fixed base point. Let $d : X \to \mathbb{R}$ be the distance function to r, i.e., $d(x) = d_X(r, x)$.

3.1 The Reeb and α-Reeb graphs of d

The Reeb graph. The relation $x \sim y$ if and only if $d(x) = d(y)$ and x, y are in the same path connected component of $d^{-1}(d(x))$ is an equivalence relation. The quotient space $G = X/\sim$ is called the *Reeb graph* of d and we denote by $\pi : X \to G$ the quotient map. Notice that π is continuous and as X is path connected, G is path connected. The function d induces a function $d_* : G \to \mathbb{R}_+$ that satisfies $d = d_* \circ \pi$. The relation defined by: for any $g, g' \in G$, $g \leqslant_G g'$ if and only if $d_*(g) \leqslant d_*(g')$ and there exist a continuous path γ in G connecting g to g' such that $d \circ \gamma$ is non decreasing, makes G a partially ordered set.

The α-Reeb graphs. Computing or approximating the Reeb graph of (X, d) from a finite set of point sampled on X is usually a difficult task. To overcome this issue we also consider a variant of the Reeb graph that shares very similar properties than the Reeb graph. Let $\alpha > 0$ and let $\mathcal{I} = \{I_i\}_i \in I$ be a covering of the range of d by open intervals of length at most α. The transitive closure of the relation $x \sim_\alpha y$ if and only if $d(x) = d(y)$ and x, y are in the same path connected component of $d^{-1}(I_i)$ for some interval $I_i \in \mathcal{I}$ is an equivalence relation that is also denoted by $\sim_\alpha$. The quotient space $G_\alpha = X/\sim_\alpha$ is called the *α-Reeb graph*[3] of d and we denote by $\pi : X \to G_\alpha$ the quotient map. Notice that π is continuous and as X is path connected, G_α is path connected. The function d induces a function $d_* : G_\alpha \to \mathbb{R}_+$ that satisfies $d = d_* \circ \pi$. The relation defined by: for any $g, g' \in G_\alpha$, $g \leqslant_{G_\alpha} g'$ if and only if $d_*(g) \leqslant d_*(g')$ and there exist a continuous path γ in G_α connecting g to g' such that $d \circ \gamma$ is non decreasing, makes G_α a partially ordered set.

The α-Reeb graph is closely related to the graph constructed by the Mapper algorithm introduced in [33] making its computation much more easier than the Reeb graph (see Section 4).

Notice that without making assumptions on X and d, in general G and G_α are not finite graphs. However when the number of path connected components of the level sets of d is finite and changes only a finite number of times then the Reeb graph turns out to be a finite directed acyclic graph. Similarly, when the covering of X by the connected components of $d^{-1}(I_i), i \in \mathcal{I}$ is finite, the α-Reeb graph also turns out to be a finite directed acyclic graph. This happens in most applications and for example when (X, d_X) is

[2] recall that a minimizing geodesic in X is any curve $\gamma : I \to X$, where I is a real interval, such that $d_X(\gamma(t), \gamma(t')) = |t - t'|$ for any $t, t' \in I$.

[3] strictly speaking we should call it the α-Reeb graph associated to the covering $\mathcal{I}$ but we assume in the sequel that some covering $\mathcal{I}$ has been chosen and we omit it in notations

a finite simplicial complex or a compact semialgebraic (or more generally a compact subanalytic space) with d being semi-algebraic (or subanalytic).

All the results and proofs presented in Section 3 are exactly the same for the Reeb and the α-Reeb graphs. In the following paragraph and in Section 3.2, G denotes indifferently the Reeb graph or an α-Reeb graph for some $\alpha > 0$. We also always assume that X and d (and α and $\mathcal{I}$) are such that G is a finite graph.

A metric on Reeb and α-Reeb graphs. Let define the set of vertices V of G as the union of the set of points of degree not equal to 2 with the set of local maxima of d_* over G, and the base point $\pi(r)$. The set of edges E of G is then the set of the connected components of the complement of V. Notice that $\pi(r)$ is the only local (and global) minimum of d_*: since X is path connected, for any $x \in X$ there exists a geodesic γ joining r to x along which d is increasing; d_* is thus also increasing along the continuous curve $\pi(\gamma)$, so $\pi(x)$ cannot be a local minimum of d_*. As a consequence d_* is monotonous along the edges of G. We can thus assign an orientation to each edge: if $e = [p, q] \in G$ is such that $d_*(p) < d_*(q)$ then the positive orientation of e is the one pointing from p to q. Finally, we assign a metric to G. Each edge $e \in E$ is homeomorphic to an interval to which we assign a length equal to the absolute difference of the function d_* at two endpoints. The distance between two points p, p' of e is then $|d_*(p) - d_*(p')|$. This makes G a metric graph (G, d_G) isometric to the quotient space of the union of the intervals isometric to the edges by identifying the endpoints if they correspond to the same vertex in G. See Figure 1 for an example. Note that d_* is continuous in (G, d_G) and for any $p \in G$, $d_*(p) = d_G(\pi(r), p)$. Indeed this is a consequence of the following lemma.

Lemma 3.1. *If δ is a path joining two points $p, p' \in G$ such that $d_* \circ \delta$ is strictly increasing then δ is a shortest path between p and p' and $d_G(p, p') = d_*(p') - d_*(p)$.*

Proof. As $d_* \circ \delta$ is strictly increasing, when δ enters an edge e by one of its end points, either it exits at the other end point or it stops at p' if $p' \in e$. Moreover δ cannot go through a given edge more than one time. As a consequence δ can be decomposed in a finite sequence of pieces $e_0 = [p, p_1], e_1 = [p_1, p_2], \cdots, e_{n-1} = [p_{n-1}, p_n], e_n = [p_n, p']$ where e_0 and e_n are the segments joining p and p' to one of the endpoint of the edges that contain them and $e_1, \cdots, e_{n-1}$ are edges. So, the length of δ is equal to $(d_*(p_1) - d_*(p)) + (d_*(p_2) - d_*(p_1)) + \cdots + (d_*(p') - d_*(p_n)) = d_*(p') - d_*(p)$ and $d_G(p, p') \leqslant d_*(p') - d_*(p)$.

Similarly any simple path joining p to p' can be decomposed in a finite sequence of pieces $e'_0 = [p, p'_1], e'_1 = [p'_1, p'_2], \cdots, e'_{k-1} = [p'_{k-1}, p'_k], e'_k = [p'_k, p']$ where e'_0 and e'_k are the segments joining p and p' to one of the endpoint of the edges that contain them, and $e'_1, \cdots, e'_{k-1}$ are edges. Now, as we do not know that d_* is increasing along this path, its length is thus equal to $|d_*(p'_1) - d_*(p)| + |d_*(p'_2) - d_*(p'_1)| + \cdots + |d_*(p') - d_*(p'_n)| \geqslant d_*(p') - d_*(p)$. So, $d_G(p, p') \geqslant d_*(p') - d_*(p)$. □

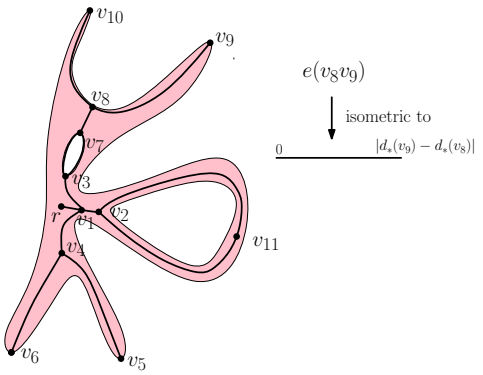


Figure 1: Construction of a Reeb graph.

3.2 Bounding the Gromov-Hausdorff distance between X and G

The goal of this section is to provide an upper bound of the Gromov-Hausdorff distance between X and G that only depends on the first Betti number $\beta_1(G)$ of G and the maximal diameter M of the level sets of π. An upper bound of M is given in the next section.

Theorem 3.2. *$d_{GH}(X,G) < (\beta_1(G)+1)M$ where $d_{GH}(X,G)$ is the Gromov-Hausdorff distance between X and G, $\beta_1(G)$ is the first Betti number of G and $M = \sup_{p\in G}\{\text{diameter}(\pi^{-1}(p))\}$ is the supremum of the diameters of the level sets of π.*

The proof of Theorem 3.2 will be easily deduced from a sequence of technical lemmas that allow to compare the distance between pair of points $x, y \in X$ and the distance between their images $\pi(x), \pi(y) \in G$.

A vertex $v \in V$ is called a *merging vertex* if it is the end point of at least two edges e_1 and e_2 that are pointing to it according to the orientation defined in Section 3.1. Geometrically this means that there are at least two distinct connected components of $\pi^{-1}(d_*^{-1}(d_*(v)-\varepsilon))$ that accumulate to $\pi^{-1}(v)$ as $\varepsilon > 0$ goes to 0. The set of merging vertices is denoted by V_m.

The following lemma provides an upper bound on the number of vertices in V_m.

Lemma 3.3. *The number of elements in V_m is equal to $\beta_1(G)$ where $\beta_1(G)$ is the first homology group of G.*

Proof. The result follows from classical homology persistence theory [20]. First remark that, as $\pi(r)$ is the only local minimum of d_*, the sublevel sets of the function $d_* : G \to \mathbb{R}_+$ are all path connected. Indeed if $\pi(x), \pi(y) \in G$ are in the same sublevel set $d_*^{-1}([0,\alpha])$, $\alpha > 0$, then the images by π of the shortest paths in X connecting x to r and y to r are contained in $d_*^{-1}([0,\alpha])$ and their union is a continuous path joining $\pi(x)$ to $\pi(y)$. As a consequence, the 0-dimensional persistence of d_* is trivial. So, for the persistence algorithm applied to d_*, the vertices of V_m are the positive simplices (see [21] for the notion of positive and negative simplices for persistence). It follows that each vertex of V_m creates a cycle that never dies as G is one dimensional and does not contain any 2-dimensional simplex. Thus $|V_m| = \beta_1(G)$. □

Lemma 3.4. *Let $p, p' \in G$ and let $\delta : [d_*(p), d_*(p')] \to G$ be a strictly increasing path going from p to p' that does not contain any point of V_m in its interior. Then for any $x' \in \pi^{-1}(p') \cap cl(\pi^{-1}(\delta(d_*(p), d_*(p'))))$ where $cl(.)$ denotes the closure, there exists a shortest path γ connecting a point x of $\pi^{-1}(p)$ to x' such that $\pi(\gamma) = \delta$ and $d_X(x,x') = d(x') - d(x) = d_*(p') - d_*(p) = d_G(p,p')$.*

Notice that from Lemma 3.1, δ is a shortest path and the parametrization by the interval $[d_*(p), d_*(p')]$ can be chosen to be an isometric embedding.

Proof. First assume that p' is not a merging point. Let $\gamma_0 : [0, d(x')] \to X$ be any shortest path between r and x' and let γ be the restriction of γ_0 to $[d_*(p), d(x')] = [d_*(p), d_*(p')]$. If the infimum t_0 of the set $I = \{t \in [d_*(p), d_*(p')] : \pi(\gamma(t')) \in \delta,\ \forall t' \geqslant t\}$ is larger than $d_*(p)$, then $\pi(\gamma(t_0))$ then there exists an increasing sequence (t_n) that converges to t_0 such that $\gamma(t_n) \notin \delta$. As a consequence $\delta(t_0)$ is a merging point; a contradiction. So $t_0 = d_*(p)$ and $\gamma(d_*(p))$ intersects $\pi^{-1}(p)$ at a point x.

Now if p' is a merging point, as x' is chosen in the closure of $\pi^{-1}(\delta(d_*(p), d_*(p'))$, for any sufficiently large $n \in \mathbb{N}$ one can consider a sequence of points $x'_n \in \pi^{-1}(\delta(d_*(p') - 1/n))$ that converges to x' and apply the first case to get a sequence of shortest path γ_n from a point $x_n \in \pi^{-1}(p)$ and x'_n. Then applying Arzelà-Ascoli's theorem (see [19] 7.5) we can extract from γ_n a sequence of points converging to a shortest path γ between a point $x \in \pi^{-1}(p)$ and x'.

To conclude the proof, notice that from Lemma 3.1 we have $d_G(p,p') = d_*(p') - d_*(p) = d(x') - d(x)$. Since γ is the restriction of a shortest path from r to x we also have $d_X(x,x') = d(x') - d(x)$. □

Lemma 3.5 and Lemma 3.6 allow to compare the metrics d_X and d_G.

Lemma 3.5. *For any $x, y \in X$ we have*

$$d_X(x,y) \leqslant d_G(\pi(x),\pi(y)) + 2(\beta_1(G)+1)M$$

where $\beta_1(G)$ is the first Betti number of G and $M = \sup_{p\in G}\{$diameter$(\pi^{-1}(p))\}$.

Proof. Let δ be a shortest path between $\pi(x)$ and $\pi(y)$. Remark that except at the points $\pi(x)$ and $\pi(y)$ the local maxima of the restriction of d_* to δ are in V_m. Indeed as δ is a shortest path it has to be simple, so if $p \in \delta$ is a local maximum then p has to be a vertex and δ has to pass through two edges having p as end point and pointing to p according to the orientation defined in Section 3.1. So p is a merging point. Since δ is simple and V_m is finite, δ can be decomposed in at most $|V_m|+1$ connected paths along the interior of which the restriction of d_* does not have any local maxima. So along each of these connected paths the restriction of d_* can have at most one local minimum. As a consequence, δ can be decomposed in a finite number of continuous paths $\delta_1, \delta_2, \cdots, \delta_k$ with $k \leqslant 2(|V_m|+1)$, such that the restriction of d_* to each of these path is strictly monotonous. For any $i \in \{1, \cdots, k\}$ let p_i and p_{i+1} the end points of δ_i with $p_1 = \pi(x)$ and $p_{k+1} = \pi(y)$. We can apply Lemma 3.4 to each δ_i to get a shortest path γ_i in X between a point $x_i \in \pi^{-1}(p_i)$ and a point in $y_{i+1} \in \pi^{-1}(p_{i+1})$ such that $\pi(\gamma_i) = \delta_i$ and $d_X(x_i, y_{i+1}) = d_G(p_i, p_{i+1})$. The sum of the lengths of the paths γ_i is equal to the sum of the lengths of the path δ_i which is itself equal to $d_G(\pi(x),\pi(y))$. Now for any $i \in \{1, \cdots, k\}$, since $\pi(x_i) = \pi(y_i)$ we have $d_X(x_i, y_i) \leqslant M$ and x_i and y_i can be connected by a path of length at most M (x_1 is connected to x and y_{k+1} is connected to y. Gluing these paths to the paths γ_i gives a continuous path from x to y whose length is at most $d_G(\pi(x),\pi(y)) + kM \leqslant d_G(\pi(x),\pi(y)) + 2(|V_m|+1)M$. Since from Lemma 3.3, $|V_m| \leqslant \beta_1(G)$, we finally get that $d_X(x,y) \leqslant d_G(\pi(x),\pi(y)) + 2(\beta(G)+1)M$. □

Lemma 3.6. *The map $\pi : X \to G$ is 1-Lipschitz: for any $x, y \in X$ we have*

$$d_G(\pi(x),\pi(y)) \leqslant d_X(x,y).$$

Proof. Let $x, y \in X$ and let $\gamma : I \to X$ be a shortest path from x to y in X where $I \subset \mathbb{R}$ is a closed interval. The path $\pi(\gamma)$ connects $\pi(x)$ and $\pi(y)$ in G.

We first claim that there exists a continuous path Γ contained in $\pi(\gamma)$ connecting $\pi(x)$ and $\pi(y)$ that intersects each vertex of G at most one time. The path Γ can be defined by iteration in the following way. Let $v_1, \cdots v_n \in V$ be the vertices of G that are contained in $\pi(\gamma) \setminus \{\pi(x), \pi(y)\}$ and let $\Gamma_0 = \pi(\gamma) : J_0 = I \to G$. For $i = 1, \cdots n$ let $t_i^- = \inf\{t : \Gamma_{i-1}(t) = v_i\}$ and $t_i^+ = \sup\{t : \Gamma_{i-1}(t) = v_i\}$ and define Γ_i as the restriction of Γ_{i-1} to $J_i = J_{i-1} \setminus (t_i^-, t_i^+)$. The path Γ_i is a connected continuous path (although J_i is a disjoint union of intervals) that intersects the vertices $v_1, v_2, \cdots, v_i$ at most one time. We then define $\Gamma = \Gamma_n : J = J_n \to G$ where $J \subset I$ is a finite union of closed intervals. Notice that Γ is the image by π of the restriction of γ to J and that $\Gamma(t) \in \{v_1, \cdots v_n\}$ only if t is one of the endpoints of the closed intervals defining J.

Now, for each connected component $[t,t']$ of J, $\gamma((t,t'))$ is contained in $\pi^{-1}(e)$ where e is the edge of G containing $\Gamma([t,t'])$. As a consequence, $d_G(\pi(\gamma)(t), \pi(\gamma)(t')) = |d_*(\pi(\gamma)(t) - d_*(\pi(\gamma)(t'))| = |d(\gamma(t)) - d(\gamma(t'))|$. Recalling that $d(\gamma(t)) = d_X(r, \gamma(t))$ and $d(\gamma(t')) = d_X(r, \gamma(t'))$ and using the triangle inequality we get that $|d(\gamma(t)) - d(\gamma(t'))| \leqslant d_X(\gamma(t), \gamma(t'))$. To conclude the proof, since γ is a geodesic path we just need to sum up the previous inequality over all connected components of J:

$$d_X(x,y) \geqslant \sum_{[t,t']\in cc(J)} d_X(\gamma(t),\gamma(t')) \geqslant \sum_{[t,t']\in cc(J)} d_G(\pi(\gamma)(t), \pi(\gamma)(t')) \geqslant d_G(\pi(x),\pi(y))$$

where $cc(J)$ is the set of connected components of J. □

The proof of Theorem 3.2 now easily follows from Lemmas 3.5 and 3.6.

Proof. (of Theorem 3.2) Consider the set $C = \{(x, \pi(x)) : x \in X\} \subset X \times G$. As π is surjective this is a correspondence between X and G. It follows from Lemmas 3.5 and 3.6 that for any $(x,\pi(x)), (y,\pi(y)) \in C$,

$$|d_X(x,y) - d_G(\pi(x),\pi(y))| \leqslant 2(\beta_1(G)+1)M$$

where $\beta_1(G)$ is the first Betti number of G and $M = \sup_{p\in G}\{\text{diameter}(\pi^{-1}(p))\}$. So C is a $(2(\beta_1(G)+1)M$-correspondence and $d_{GH}(X,G) \leqslant (\beta_1(G)+1)M$. □

3.3 Bounding M

To upperbound the diameter of the level sets of π we first prove the two following general lemmas.

Lemma 3.7. *Let (G, d_G) be a connected finite metric graph and let $r \in G$. We denote by $d_r = d_G(r,.) : G \to [0,+\infty)$ the distance to r. For any edge $E \subset G$, the restriction of d_r to e is either strictly monotonous or has only one local maximum. Moreover the length $l = l(E)$ of E is upper bounded by two times the difference between the maximum and the minimum of d_r restricted to E.*

Proof. Let l be the length of E and let $t \mapsto e(t)$, $t \in [0,l]$, be an arc length parametrization of E. Since E is an edge of G, for $t \in [0,l]$ any shortest geodesic γ_t joining r to $e(t)$ must contain either $x_1 = e(0)$ or $x_2 = e(l)$. If it contains x_1 then for any $t' < t$ the restriction of γ_t between r and $e(t')$ is a shortest geodesic containing x_1 and if it contains x_2 then for any $t' > t$ the restriction of γ_t between r and $e(t')$ is a shortest geodesic containing x_2. Moreover in both cases, the function d_r is strictly monotonous along γ. As a consequence, the set $I_1 = \{t \in [0,l] : \text{a shortest geodesic joining } r \text{ to } e(t) \text{ contains } x_1\}$ is a closed interval containing 0. Similarly the set $I_2 = \{t \in [0,l] : \text{a shortest geodesic joining } r \text{ to } e(t) \text{ contains } x_2\}$ is a closed interval containing l and $[0,l] = I_1 \cup I_2$. Moreover d_r is strictly monotonous on $e(I_1)$ and on $e(I_2)$. As a consequence $I_1 \cap I_2$ is reduced to a single point t_0 that has to be the unique local maximum of d_r restricted to E.

The second part of the lemma follows easily from the previous proof: the minimum of d_r restricted to E is attained either at x_1 or x_2 and $d_r(e(t_0)) = d_r(x_1) + t_0 = d_r(x_2) + l - t_0$ is the maximum of d_r restricted to E. We thus obtain that $2t_0 = l + (d_r(x_2) - d_r(x_1))$. As a consequence if $d_r(x_1) \leqslant d_r(x_2)$ then $l/2 \leqslant t_0 = d_r(e(t_0)) - d_r(x_1)$; similarly if $d_r(x_1) \geqslant d_r(x_2)$ then $l/2 \leqslant l - t_0 = d_r(e(t_0)) - d_r(x_2)$. □

Lemma 3.8. *Let (G, d_G) be a connected finite metric graph and let $r \in G$. For $\alpha > 0$ we denote by $N_E(\alpha)$ the number of edges of G of length at most α. For any $d > 0$ and any connected component B of the set $B_{d,\alpha} = \{x \in G : d - \alpha \leqslant d_G(r,x) \leqslant d + \alpha\}$ we have*

$$diam(B) \leqslant 4(2 + N_E(4\alpha))\alpha$$

The example of figure 2 shows that the bound of Lemma 3.8 is tight.

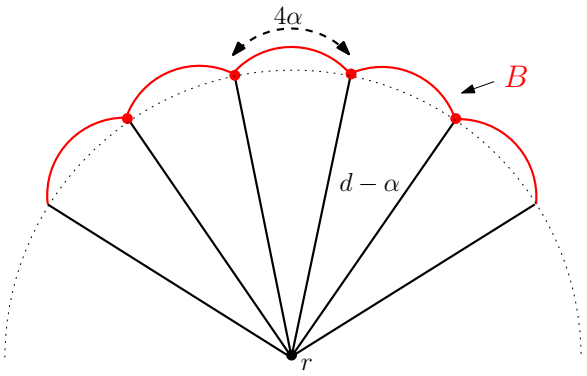


Figure 2: Tightness of the bound in Lemma 3.8: there are 3 edges of length at most 4α and the diameter of B is equal to 20α.

Proof. Let $x, y \in B$ and let $t \mapsto \gamma(t) \in B$ be a continuous path joining x to y in B. Let E be an edge of G that does not contain x or y and with end points x_1, x_2 such that γ intersects the interior of E. Then $\gamma^{-1}(E)$ is a disjoint union of closed intervals of the form $I = [t,t']$ where $\gamma(t)$ and $\gamma(t')$ belong to the

set $\{x_1, x_2\}$. If $\gamma(t) = \gamma(t')$ we can remove the part of γ between t and t' and still get a continuous path between x and y. So without loss of generality we can assume that if γ intersects the interior of E, then E is contained in γ. Using the same argument as previously we can also assume that if γ goes across E, it only does it one time, i.e. $\gamma^{-1}(E)$ is reduced to only one interval. As a consequence, γ can be decomposed in a sequence $[x, v_0], E_1, E_2, \cdot, E_k, [v_k, y]$ where $[x, v_0]$ and $[v_k, y]$ are pieces of edges containing x and y respectively and $E_1 = [v_0, v_1], E_2 = [v_1, v_2]\cdot, E_k = [v_{k-1}, v_k]$ are pairwise distinct edges of G contained in B. It follows from Lemma 3.7 that the lengths of the edges $E_1, \cdots E_k$ and of $[x, v_0]$ and $[v_k, y]$ are upper bounded by 4α. As a consequence the length of γ is upper bounded by $4(k+2)\alpha$ which is itself upper bounded by $4(N_E(4\alpha)+2)\alpha$ since the edges $E_1, \cdots E_k$ are pairwise distinct. It follows that $d_G(x, y) \leqslant 4(N_E(4\alpha)+2)\alpha$. □

Theorem 3.9. *Let (G, d_G) be a connected finite metric graph and let (X, d_X) be a compact geodesic metric space such that $d_{GH}(X, G) < \varepsilon$ for some $\varepsilon > 0$. Let $x_0 \in X$ be a fixed point and let $d_{x_0} = d_X(x_0, .) : X \to [0, +\infty)$ be the distance function to x_0. Then for $d \geqslant \alpha \geqslant 0$ the diameter of any connected component L of $d_{x_0}^{-1}([d-\alpha, d+\alpha])$ satisfies*

$$diam(L) \leqslant 4(2 + N_E(4(\alpha + 2\varepsilon)))(\alpha + 2\varepsilon) + \varepsilon$$

where $N_E(4(\alpha+2\varepsilon))$ is the number of edges of G of length at most $4(\alpha+2\varepsilon)$. In particular if $\alpha = 0$ and 8ε is smaller that the length of the shortest edge of G then the diameter of L is upper bounded by 17ε.

Proof. Let $\varepsilon' > 0$ be such that $d_{GH}(X, G) < \varepsilon' < \varepsilon$. Let $C \subset X \times G$ be an ε'-correspondence between X and G and $(x_0, r) \in C$. we denote by $d_r = d_G(r, .) : G \to [0, +\infty)$ the distance function to r in G. Let $x_a, x_b \in L$ and let $(x_a, y_a), (x_b, y_b) \in C$. There exists a continuous path $\gamma \subseteq L$ joining x_a to x_b. Since C is an ε'-correspondence for any $x \in \gamma$ there exists a point $(x, y) \in C$ such that $d - \alpha - \varepsilon' \leqslant d_r(y) \leqslant d+\alpha+\varepsilon'$. The set of points y obtained in this way is not necessarily a continuous path from y_a to y_b. However one can consider a finite sequence $x_1 = x_a, x_2, \cdots, x_n = x_b$ of points in γ such that for any $i = 1, \cdots n-1$ we have $d_X(x_i, x_{i+1}) < \varepsilon - \varepsilon'$. If $(x_i, y_i) \in C$ then we have $d_G(y_i, y_{i+1}) < \varepsilon - \varepsilon' + \varepsilon' = \varepsilon$. As a consequence, since $d - \alpha - \varepsilon < d - \alpha - \varepsilon' < d_r(y_i) < d + \alpha + \varepsilon' < d + \alpha + \varepsilon$ the shortest geodesic connecting y_i to y_{i+1} in G remains in the set $d_r^{-1}([d-\alpha-2\varepsilon, d+\alpha+2\varepsilon])$ and connecting these geodesics for all $i = 1, \cdots, n-1$ we get a continuous path from y_a to y_b in $d_r^{-1}([d-\alpha-2\varepsilon, d+\alpha+2\varepsilon])$. It then follows from Proposition 3.8 that $d_G(y_a, y_b) \leqslant\leqslant 4(2 + N_E(4(\alpha+2\varepsilon)))(\alpha+2\varepsilon)$ and since C is an ε'-correspondence (and so an ε-correspondence), $d_X(x_a, x_b) < 4(2 + N_E(4(\alpha+2\varepsilon)))(\alpha+2\varepsilon) + \varepsilon$. □

As a corollary of the Theorem 3.9 and Theorem 3.2 we immediately obtain the following results for the Reeb graph and the α-Reeb graphs.

Theorem 3.10. *Let (X, d_X) be a compact connected path metric space, let $r \in X$ be a fixed base point such that the metric Reeb graph (G, d_G) of the function $d = d_X(r, .) : X \to \mathbb{R}$ is a finite graph. If for a given $\varepsilon > 0$ there exists a finite metric graph $(G', d_{G'})$ such that $d_{GH}(X, G') < \varepsilon$ then we have*

$$d_{GH}(X, G) < (\beta_1(G) + 1)(17 + 8N_{E,G'}(8\varepsilon))\varepsilon$$

where $N_{E,G'}(8\varepsilon)$ is the number of edges of G' of length at most 8ε. In particular if X is at distance less than ε from a metric graph with shortest edge length larger than 8ε then $d_{GH}(X, G) < 17(\beta_1(G)+1)\varepsilon$.

Theorem 3.11. *Let (X, d_X) be a compact connected path metric space. Let $r \in X$, $\alpha > 0$ and $\mathcal{I}$ be a finite covering of the segment $[0, Diam(X)]$ by open intervals of length at most α such that the α-Reeb graph G_α associated to $\mathcal{I}$ and the function $d = d_X(r, .) : X \to \mathbb{R}$ is a finite graph. If for a given $\varepsilon > 0$ there exists a finite metric graph $(G', d_{G'})$ such that $d_{GH}(X, G') < \varepsilon$ then we have*

$$d_{GH}(X, G_\alpha) < (\beta_1(G_\alpha) + 1)(4(2 + N_{E,G'}(4(\alpha+2\varepsilon)))(\alpha+2\varepsilon) + \varepsilon)$$

where $N_{E,G'}(4(\alpha+2\varepsilon))$ is the number of edges of G' of length at most $4(\alpha+2\varepsilon)$. In particular if X is at distance less than ε from a metric graph with shortest edge length larger than $4(\alpha+2\varepsilon)$ then $d_{GH}(X, G_\alpha) < (\beta_1(G_\alpha)+1)(8\alpha + 17\varepsilon)$.

4 Algorithm

In this section, we describe an algorithm for computing α-Reeb graph for some $\alpha > 0$. We assume the input of the algorithm is a neighboring graph $H = (V, E)$, a function $l : E \to \mathbb{R}^+$ specifying the edge length and a parameter α. In the applications where the input is given as a set of points together with pairwise distances, i.e., a finite metric space, one can generate the neighboring graph H as a Rips graph of the input points with the parameter chosen as a fraction of α.

Our algorithm can be described as follows. We assume H is connected as one can apply the algorithm to each connected component if H is not . Figure 3 illustrates the different steps of the algorithm. In the first step, we fix a node of H as the root r and then obtain the distance function $d : V \to \mathbb{R}^+$ by computing $d(v)$ as the graph distance from the node v to r. In the second step, we apply the Mapper algorithm [33] to the nodes V with filter d to construct a graph $\tilde{G}$. Specifically, let $\mathcal{I} = \{(i\alpha, (i+1)\alpha), ((i+0.5)\alpha, (i+1.5)\alpha) | 0 \leqslant i \leqslant m\}$ so that $\cup_{I_k \in \mathcal{I}} I_k$ covers the range of the function d. We say an interval $I_{k_1} \in \mathcal{I}$ is lower than another interval $I_{k_2} \in \mathcal{I}$ if the midpoint of I_{k_1} is smaller than that of I_{k_2}. Now let H_k be the subgraph of H restricted to $V_k = d^{-1}(I_k)$. Namely two nodes in H_k are connected with an edge if they are in H. Notice that each subgraph H_k may have several connected components, which can be listed in an arbitrary order. Denote H_k^l the l-th connected component of H_k and V_k^l its set of nodes. Think of $\{V_k^l\}_{k,l}$ as a cover of V. Then the graph $\tilde{G}$ constructed by the Mapper algorithm is the 1-skeleton of the nerve of that cover. Namely, each node in $\tilde{G}$ represents an element in $\{V_k^l\}_{k,l}$, i.e., a subset of nodes in V. Two nodes $V_{k_1}^{l_1}$ and $V_{k_2}^{l_2}$ are connected with an edge if $V_{k_1}^{l_1} \cap V_{k_2}^{l_2} \neq \emptyset$.

In the final step, we represent each node V_k^l in $\tilde{G}$ using a copy of the interval I_k. As mentioned in the Section 3.1, α-Reeb graph is a quotient space of the disjoint union of those copies of intervals. Specifically, for an edge in $\tilde{G}$, let $V_{k_1}^{l_1}$ and $V_{k_2}^{l_2}$ be its endpoints. Then I_{k_1} and I_{k_2} must be partially overlapped. We identify the overlap part of these two intervals. After identifying the overlapped intervals for all edges in $\tilde{G}$, the resulting quotient space is the α-Reeb graph. Algorithmically, the identification is performed as follows. We split each copy of internal I_k into two by adding a point in the middle. Now think of it as a graph with two edges and label one of them upper and the other lower. Notice that two overlapped intervals I_{k_1} and I_{k_2} can not be exactly the same. One must be lower than the other. To identify their overlapped part, we identify the upper edge of the lower interval with the lower edge of the upper interval.

The time complexity of the above algorithm is dominated by the computation of the distance function in the first step, which is $O(|E| + |V| \log |V|)$. The computation of the connected components in the second step is $O(|V| \log |V|)$ based on union-find data structure. In the final step, there are at most $O(|V|)$ number of the copies of the intervals. Based on union-find data structure, the identification can also be performed in $O(|V| \log |V|)$ time.

5 Experiments

In this section, we apply our algorithm to a few data sets. The first data set is that of earthquake locations through which we wish to learn the geometric information about earthquake faults. The raw data was obtained from USGS Earthquake Search [32] and consists of earthquakes between 01/01/1970 and 01/01/2010, of magnitude greater than 5.0, and of location in the rectangular area between latitudes -75 degrees and 75 degrees and longitude between -170 degrees and 10 degrees. The raw earthquake data set contains the coordinates of the epicenters of 12790 earthquakes. We follow the procedure described in [1] to remove outliers and randomly sampled 1600 landmarks. Finally, we computed a neighboring graph from these landmarks with parameter 4. The length of an edge in this graph is the Euclidean distance between its endpoints. For each connected component, we fix a root point and compute the graph distance function d to the root point as shown in Figure 4(a). Set α also equals 4 and apply our algorithm to the above data to obtain the α-Reeb graph. In general α-Reeb graph is an abstract metric graph. In this example, for the purpose of visualization, we use the coordinates of the landmarks to embed the graph into the plane as follows. Recall that for a copy of interval I_k representing the node V_k^l in $\tilde{G}$, we split

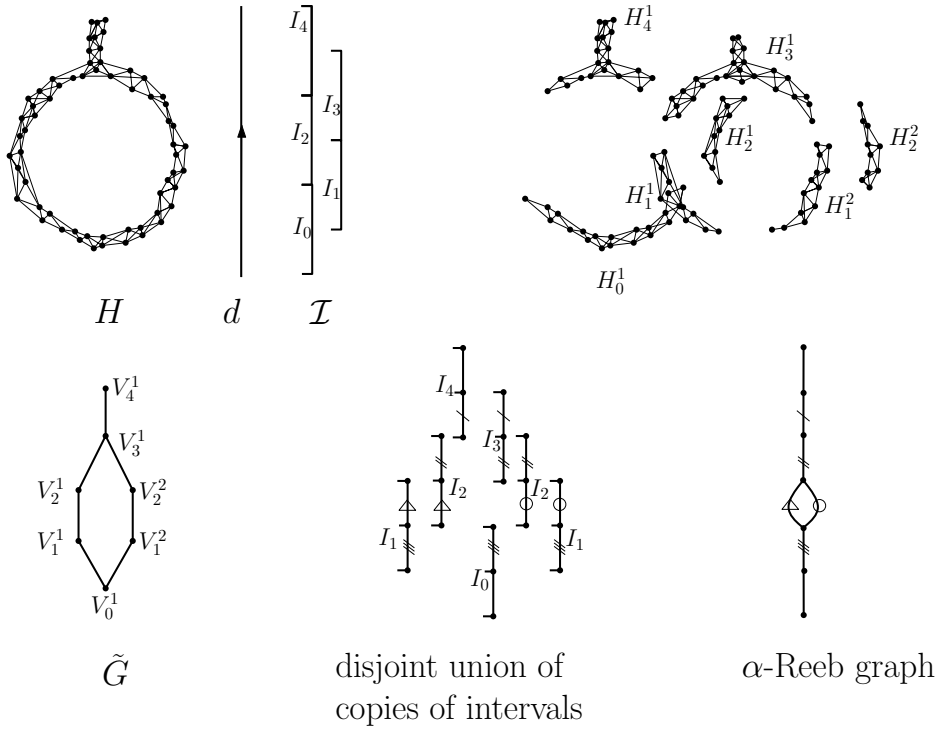


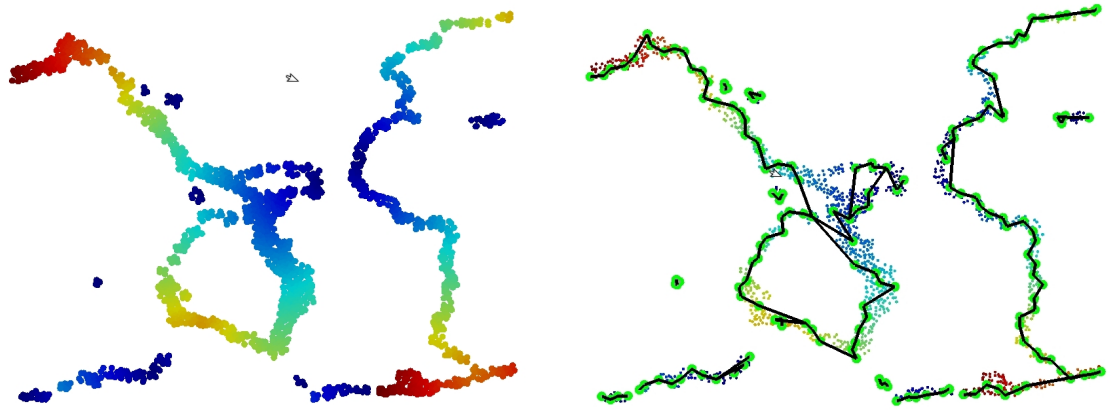
Figure 3: Illustration of the different steps of the algorithm for computing α-Reeb graph. In the disjoint union of copies of intervals, the subintervals marked with same labels are identified in the α-Reeb graph.

it into two by adding a point in the middle. We embed the endpoints of the interval to the landmarks of the minimum and the maximum of the funciton d in V_k^l, and the point in the middle to the landmark of the median of the function d in V_k^l. Figure 4(b) shows the embedding of the α-Reeb graph. Note this embedding may introduce metric distortion, i.e., the Euclidean length of the edge may not reflect the length of the corresponding edge in the α-Reeb graph.

The second data set is that of 500 GPS traces tagged "Moscow" from OpenStreetMap [30]. Since cars move on roads, we expect the locations of cars to provide information about the metric graph structure of the Moscow road network. We first selected a metric ϵ-net on the raw GPS locations with $\epsilon = 0.0001$ using furthest point sampling. Then, we computed a neighboring graph from the samples with parameter 0.0004. Again for each connected component, we fix a root point and compute the graph distance function d to the root point as shown in Figure 5(a). Set α also equals 0.0004 and compute the α-Reeb graph. Again, we use the same method as above to embed the α-Reeb graph into the plane, as shown in Figure 5(b).

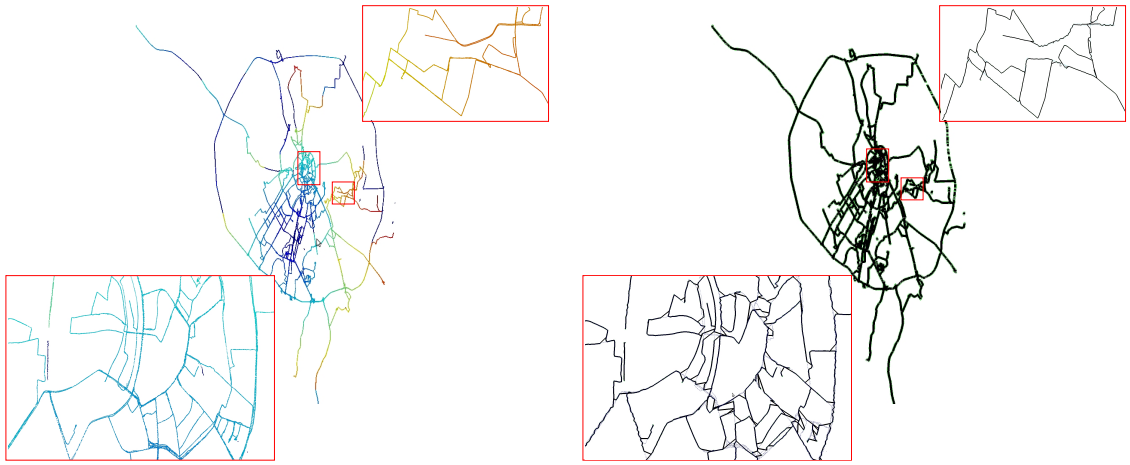
To evaluate the quality of our α-Reeb graph for each data set, we computed both original pairwise distances, and pairwise distances approximated from the constructed α-Reeb graph. For GPS traces, we randomly select 100 points as the data set is too big to compute all pairwise distances. We also evaluated the use of α-Reeb graph to speed up distance computations by showing reductions in computation time. Only pairs of points in the same connected component are included because we obtain zero error for the pairs of vertices that are not. Statistics for the size of the reconstructed graph, error of approximate distances, and reduction in computation time are given in Table 1.

Road network is directional. There are one-way streets. In fact, roads are often split so that cars in different directions run in different lanes. In particular, this is the true for highways. In addition, when two roads cross in GPS coordinates, they may bypass through a tunnel or an evaluated bridge and thus the road network itself may not cross. Since in most circumstances, drivers follow the road network and do not drive against the traffic, such directional information is contained in the GPS traces. Here we encode the directional information by stacking several consecutive GPS coordinates to form a point in



(a) (b)

Figure 4: (a) The distance functions d on each connected components. The value increases from cold to warm colors. (b) The reconstructed α-Reeb graph.



(a) (b)

Figure 5: (a) The distance functions d on each connected components. The value increases from cold to warm colors. (b) The reconstructed α-Reeb graph.

a higher dimensional space. In this way, we obtain a new set of points in this higher dimension space. Then we build a neighboring graph for this new set of points based on L_2 norm and apply our algorithm to recover the road network. In particular, although the paths intersect at the cross in GPS cooridnates, the roadnet work does not.

We first test the above strategy on a synthetic dataset, where we simulate a car driving on a highway crossing according to the right-driving rule as shown in Figure 6(a). 300 hundred traces are obtained, each of which contains 500 points. Stack 10 consecutive points along a trace to form a point in 20-dimensional space. In this way, obtain a point set in 20-dimensional space. Build a neighboring graph over this set of points where the length of an edge is the Euclidean distance of its endpoints, and compute the distance function as the graph distance to an arbitrarily chosen point as shown in Figure 6(b) where the points are projected to three space using the 1st, 2nd and 17th coordinates. To visualize the reconstructed α-Reeb graph, we choose the landmarks in the same way as the previous examples and then project them using the above three coordinates. Figure 6(c) and (d) show the reconstructed graph in two viewpoints. As we can see, we recover the road network.

Next we extract those GPS traces from the above "Moscow" dataset which pass through a highway

	GPS traces	Earthquake
#Original points	82541	1600
#Original edges	313415	26996
#Nodes in α-Reeb graph	21644	147
#Edges in α-Reeb graph	21554	137
Graph reconstruction time	46.8	0.32
Original Dist Comp Time	15.27	1.12
Approx Dist Comp Time	0.96	0.01
Mean distortion	6.5%	14.1%
Median distortion	5.3%	12.5%

Table 1: The graph reconstruction time is the total time of computing distance function and reconstructing the graph. The original distance computation time shows the total time of computing these distances using the original graph. The approximate distance computation time is the total time to compute approximate distances based on the reconstructed α-Reeb graph. All times are in seconds.

crossing as shown in Figure 7(a). Since GPS records the position based on time, we resample the traces so that the distances between any two consecutive samples is the same among all traces. Then we apply the above algorithm to the resampled traces. Figure 7(c) and (d) show the reconstructed graph which recovers the road network of this highway crossing.

6 Discussion

We have proposed a method to approximate path metric spaces using metric graphs with bounded Gromov-Hausdorff distortion, and illustrated the performances of our method on a few synthetic and real data sets. Here we point out a few possible directions for future work. First, notice that the α-Reeb graph is a quotient space where the quotient map is 1-Lipschitz and thus the metric only gets contracted. In addition, the distance from a point to the chosen root is exactly preserved. Therefore, one always reduces the metric distortion by taking the maximum of the graph metrics of different root points. It is interesting to study the strategy of sampling root points to obtain the smallest metric distortion with the fixed number of root points. Second, our method in the current form does not recover the topology of the underlying metric space. The tools recently developed in persistence homology seem useful for recovering topology: we provide a preliminary persistence-based result in the Appendix showing that the first Betti number of the underlying metric graph can be inferred from the data. On another hand, Reeb graphs have recently been used for topological inference purpose in [15]. It would be interesting to combine our method to these approaches to also obtained topologically correct reconstruction algorithms. Finally, our method is sensitive to the noise. One can of course preprocess the data and remove the noise and then apply our algorithm. Nevertheless, it is interesting to see if the algorithm can be improved to handle noise.

Acknowledgments

The authors acknowledge Daniel Müllner and G. Carlsson for fruitful discussions and for providing code for the Mapper algorithm. They acknowledge the European project CG-Learning EC contract No. 255827; the ANR project GIGA (ANR-09-BLAN-0331-01); The National Basic Research Program of China (973 Program 2012CB825501); Tsinghua National Laboratory for Information Science and TechnologyTNListCross-discipline Foundation.

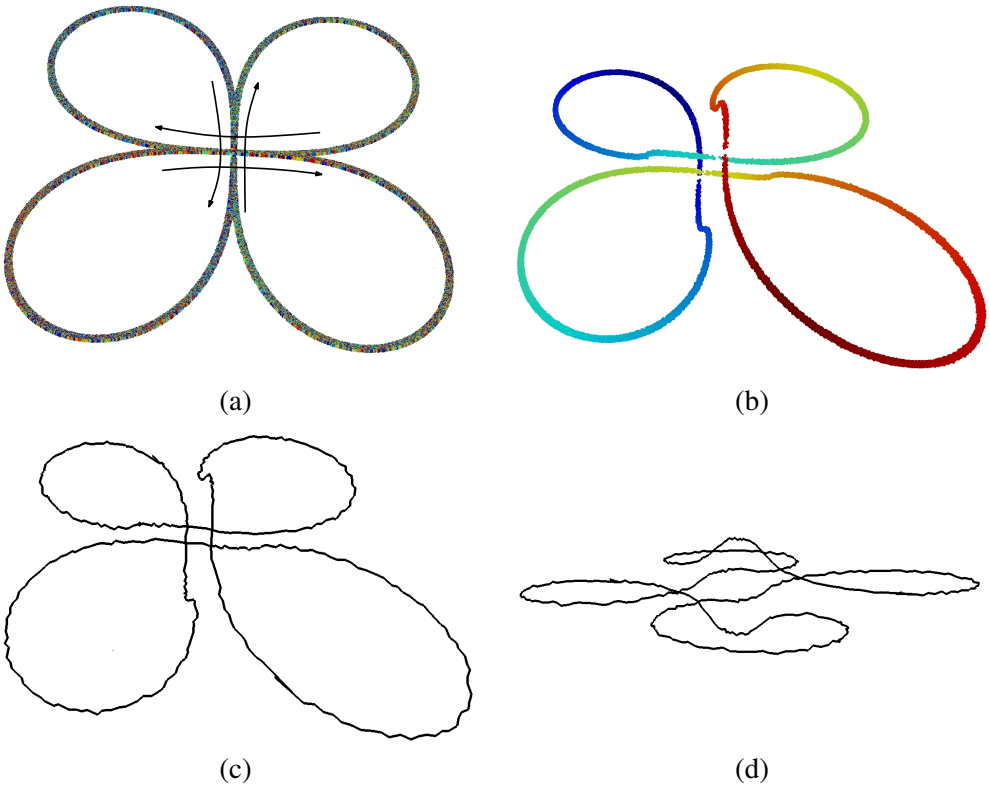


Figure 6: (a) A highway crossing and the synthetic traces. (b) The distance function. (c) and (d) The reconstructed α-Reeb graph viewed from two perspectives.

References

[1] M. Aanjaneya, F. Chazal, D. Chen, M. Glisse, L. Guibas, and D. Morozov. Metric graph reconstruction from noisy data. *International Journal of Computational Geometry & Applications*, 22(04):305–325, 2012.

[2] Ittai Abraham, Mahesh Balakrishnan, Fabian Kuhn, Dahlia Malkhi, Venugopalan Ramasubramanian, and Kunal Talwar. Reconstructing approximate tree metrics. In *PODC*, pages 43–52, 2007.

[3] Nina Amenta, Marshall Bern, and David Eppstein. The crust and the β-skeleton: Combinatorial curve reconstruction. *Graph. Models Image Process.*, 60(2):125–135, 1998.

[4] Ery Arias-Castro, David L. Donoho, , and Xiaoming Huo. Adaptive multiscale detection of filamentary structures in a background of uniform random points. *Annals of Statistics*, 34(1):326–349, 2006.

[5] M. Belkin and P. Niyogi. Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Computation*, 15(6):1373–1396, 2003.

[6] D. Burago, Y. Burago, and S. Ivanov. *A Course in Metric Geometry*, volume 33 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2001.

[7] Mihai Bădoiu, Piotr Indyk, and Anastasios Sidiropoulos. Approximation algorithms for embedding general metrics into trees. In *Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms*, SODA '07, pages 512–521, Philadelphia, PA, USA, 2007. Society for Industrial and Applied Mathematics.

[8] G. Carlsson. Topology and data. *AMS Bulletin*, 46(2):255–308, 2009.

[9] F. Chazal, V. de Silva, and S. Oudot. Persistence stability for geometric complexes. *arXiv:1207.3885*, 2012.

[10] Frédéric Chazal, Vin de Silva, Marc Glisse, and Steve Oudot. The structure and stability of persistence modules. *arXiv preprint arXiv:1207.3674*, 2012.

[11] Daniel Chen, Leonidas J. Guibas, John Hershberger, and Jian Sun. Road network reconstruction for organizing paths. In *Proceedings 21st ACM-SIAM Symposium on Discrete Algorithms (SODA)*, 2010.

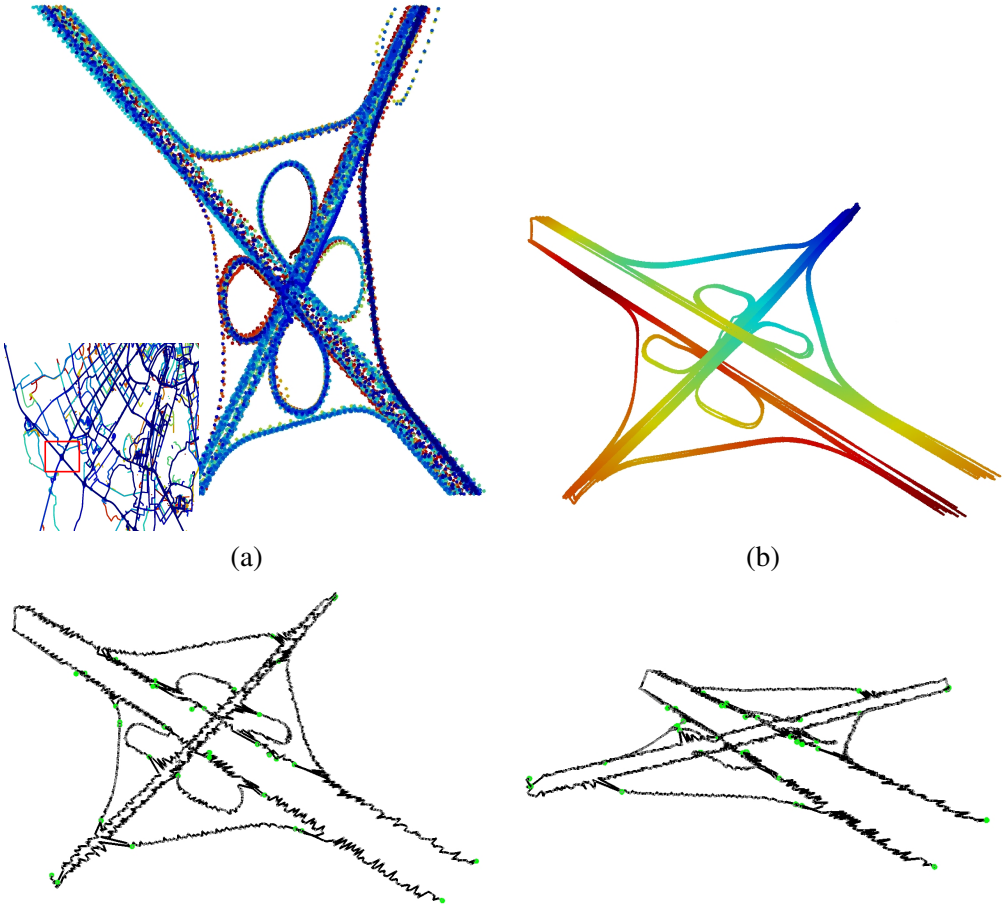


Figure 7: (a) GPS traces passing through a highway crossing in Moscow . (b) The distance function. (c) and (d)The reconstructed α-Reeb graph viewed from two perspectives.

[12] Victor Chepoi, Feodor F. Dragan, Bertrand Estellon, Michel Habib, and Yann Vaxès. Notes on diameters, centers, and approximating trees of delta-hyperbolic geodesic spaces and graphs. *Electronic Notes in Discrete Mathematics*, 31:231–234, 2008.

[13] E. Choi, N. A. Bond, M. A. Strauss, A. L. Coil, M. Davis, and C. N. A. Willmer. Tracing the filamentary structure of the galaxy distribution at $z \sim 0.8$. *Monthly Notices of the Royal Astronomical Society*, pages 692–+, May 2010.

[14] T. K. Dey, F. Fan, and Y. Wang. Graph induced complex on point data. In *Proc. 29th Annu. ACM Sympos. on Comput. Geom.*, June 2013.

[15] T. K. Dey and Y. Wang. Reeb graphs: approximation and persistence. *Discrete and Computational Geometry*, 49:46–73, 2013.

[16] Tamal K. Dey, Kurt Mehlhorn, and Edgar A. Ramos. Curve reconstruction: Connecting dots with good reason. In *Proceedings of the Fifteenth Annual Symposium on Computational Geometry*, pages 197–206. ACM, 1999.

[17] Tamal K. Dey and Rephael Wenger. Reconstructing curves with sharp corners. *Comput. Geom. Theory Appl.*, 19:89–99, July 2001.

[18] Kedar Dhamdhere, Anupam Gupta, and Harald Räcke. Improved embeddings of graph metrics into random trees. In *Proceedings of the seventeenth annual ACM-SIAM symposium on Discrete algorithm*, SODA '06, pages 61–69, New York, NY, USA, 2006. ACM.

[19] J. Dieudonné. *Foundations of Modern analysis, Volume 1*. Academic Press, 1969.

[20] H. Edelsbrunner and J. Harer. *Computational Topology: an Introduction*. American Mathematical Society, Providence, RI, 2010.

[21] H. Edelsbrunner, D. Letscher, and A. Zomorodian. Topological persistence and simplification. *Discrete Comput. Geom.*, 28:511–533, 2002.

[22] Jittat Fakcharoenphol, Satish Rao, and Kunal Talwar. A tight bound on approximating arbitrary metrics by tree metrics. In *Proceedings of the thirty-fifth annual ACM symposium on Theory of computing*, STOC '03, pages 448–455, New York, NY, USA, 2003. ACM.

[23] C. R. Genovese, M. Perone-Pacifico, I. Verdinelli, and L. Wasserman. The Geometry of Nonparametric Filament Estimation. *J. Amer. Statist. Assoc.*, (107):788–799, 2012.

[24] Christopher R. Genovese, Marco Perone-Pacifico, Isabella Verdinelli, and Larry Wasserman. On the path density of a gradient field. *Annals of Statistics*, 37(6A):3236–3271, 2009.

[25] Christopher R. Genovese, Marco Perone-Pacifico, Isabella Verdinelli, and Larry Wasserman. Nonparametric ridge estimation. *arXiv:1212.5156*, 2012.

[26] M. Gromov. *Metric Structures for Riemannian and Non-Riemannian Spaces*. Birkhäuser, 2nd edition, 2007.

[27] William Harvey, Yusu Wang, and Rephael Wenger. A randomized o(m log m) time algorithm for computing reeb graph of arbitrary simplicial complexes. In *Proc. 26th Annu. ACM Sympos. on Comput. Geom.*, 2010.

[28] J.C. Haussmann. On the vietoris-rips complexes and a cohomology theory fo metric spaces. *Ann. of Math. Stud.*, 138:175–188, 1995.

[29] S. Lafon. *Diffusion Maps and Geodesic Harmonics*. PhD. Thesis, Yale University, 2004.

[30] Openstreetmap. http://www.openstreetmap.org/.

[31] Salman Parsa. A deterministic o(m log m) time algorithm for the reeb graph. In *Proceedings of the 2012 symposuim on Computational Geometry*, SoCG '12, pages 269–276, New York, NY, USA, 2012. ACM.

[32] Earthquake search. http://earthquake.usgs.gov/earthquakes/eqarchives/epic/.

[33] G. Singh, F. Mémoli, and G. Carlsson. Topological methods for the analysis of high dimensional data sets and 3d object recognition. In *Eurographics Symposium on Point-Based Graphics*, 2007.

[34] J. B. Tenenbaum, V. De Silva, and J. C. Langford. A global geometric framework for nonlinear dimensionality reduction. *Science*, 2000.

[35] F. Tupin, H. Maitre, Mangin, Nicolas J.-F., J.-M., and E. Pechersky. Detection of linear features in SAR images: Application to road network extraction. *IEEE Transactions on Geoscience and Remote Sensing*, 36:434–453, 1998.

[36] A. Zomorodian and G. Carlsson. Computing persistent homology. *Discrete Comput. Geom.*, 33(2):249–274, 2005.

Appendix

Getting the first Betti number of a graph from an approximation

Although our metric graph reconstruction algorithm does not provide topological guarantees, we show below that, using persistent topology arguments, that the first Betti number of a graph can be inferred from an approximation.

Recall that given a compact metric space (X, d_X) and a real parameter $\alpha \geqslant 0$, the Vietoris-Rips complex $\mathrm{Rips}(X, \alpha)$ is the simplicial complex with vertex set X and whose simplices are the finite subsets of X with diameter at most α:

$$\sigma = [x_0, x_1, \cdots, x_k] \in \mathrm{Rips}(X, \alpha) \Leftrightarrow d_X(x_i, x_j) \leqslant \alpha \ \text{ forall } i, j.$$

Lemma 6.1. *Let G be a connected metric graph and let $l(G)$ be the length of the shortest loop in G that is not homologous to 0. For any metric space D such that $d_{GH}(G,D) < \frac{1}{16}l(G)$ and any $d_{GH}(G,D) < \alpha < \frac{3}{16}l(G)$, the first Betti number of G is given by*

$$b_1(G) = \text{rank}\,(H_1(\text{Rips}(D,\alpha)) \to H_1(\text{Rips}(D,3\alpha))$$

where the homomorphism between the homology groups is the one induced by the inclusion maps between the Rips complexes.

Proof. The proof follows from a result of [28] that relates the homology of the Rips complexes built on top of G to the homology of G and a result of [9] that allows to relate the Rips filtration built on top of G and D at the homology level. Since G is a geodesic path, it follows from Theorem 3.5 and Remark 2), p.179 in [28] that for any $\alpha < \frac{1}{4}l(G)$, $\text{Rips}(G,\alpha)$ and G are homotopy equivalent. Moreover, from Proposition 3.3 in [28], for any $\alpha \leqslant \alpha' < \frac{1}{4}l(G)$, the homomorphism $H_1(\text{Rips}(G,\alpha)) \to H_1(\text{Rips}(G,\alpha'))$ induced by the inclusion map is an isomorphism.

Now let $C \subset D \times G$ be an ε-correspondence between D and G where $\varepsilon < \frac{1}{16}l(G)$. According to [9], the persistence modules $(H_1(\text{Rips}(D,\alpha))_{\alpha\in\mathbb{R}_+}$ and $(H_1(\text{Rips}(G,\alpha))_{\alpha\in\mathbb{R}_+}$ are ε-interleaved. Now let α be as in the statement of the lemma and let $\beta > 0$ be such that $\beta + \varepsilon < \alpha$. The ε-interleaving induces the following sequence of homomorphisms

$$H_1(\text{Rips}(G,\beta)) \to H_1(\text{Rips}(D,\alpha)) \to H_1(\text{Rips}(G,\alpha{+}\varepsilon)) \to H_1(\text{Rips}(D,3\alpha)) \to H_1(\text{Rips}(G,3\alpha{+}\varepsilon))$$

where the composition of two consecutive homomorphisms is the homomorphism induced by the inclusion map between the corresponding Rips complexes. As a consequence since $3\alpha{+}\varepsilon < \frac{1}{4}l(G)$ the homomorphisms $H_1(\text{Rips}(G,\beta)) \to H_1(\text{Rips}(G,\alpha+\varepsilon))$ and $H_1(\text{Rips}(G,\alpha+\varepsilon)) \to H_1(\text{Rips}(G,3\alpha+\varepsilon))$ are isomorphisms of rank $b_1(G)$. It follows that the rank of $H_1(\text{Rips}(D,\alpha)) \to H_1(\text{Rips}(D,3\alpha))$ is equal to $b_1(G)$. □